



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 02:17 AM EDT

PDB ID : 1TV6 / pdb_00001tv6
Title : HIV-1 Reverse Transcriptase Complexed with CP-94,707
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Deposited on : 2004-06-28
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

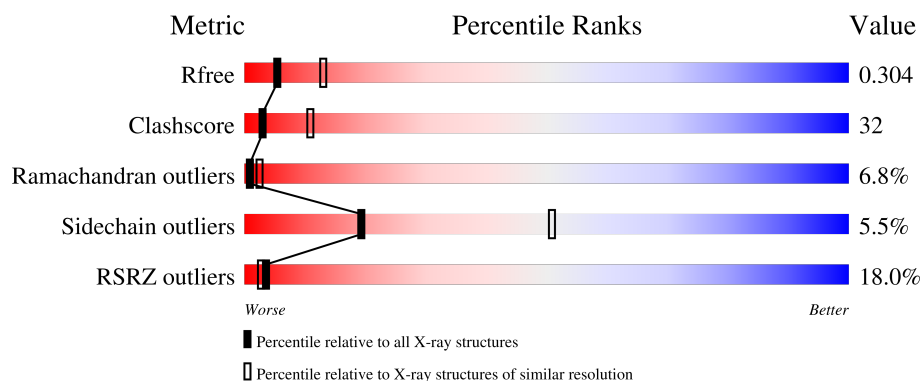
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7786 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

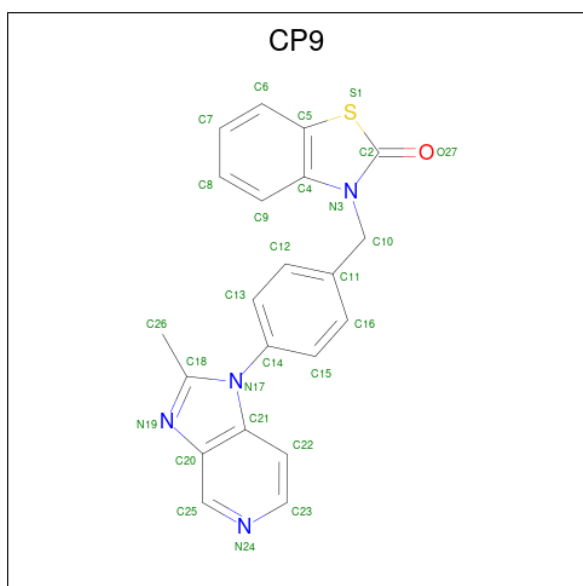
- Molecule 1 is a protein called reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4367	2832	722	805	8			

- Molecule 2 is a protein called reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	0	0	0
			3392	2205	562	618	7			

- Molecule 3 is 3-[4-(2-METHYL-IMIDAZO[4,5-C]PYRIDIN-1-YL)BENZYL]-3H-BENZOTHIADIAZOL-2-ONE (CCD ID: CP9) (formula: C₂₁H₁₆N₄OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	21	4	1	1		

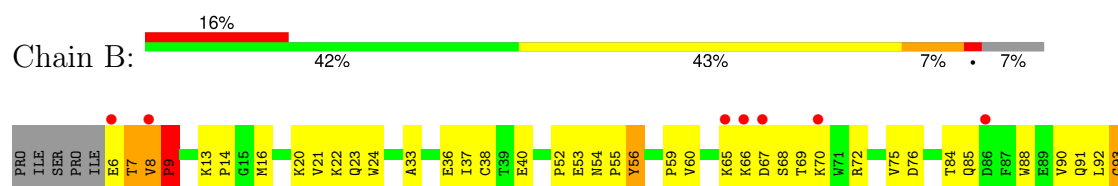
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: reverse transcriptase p66 subunit



• Molecule 2: reverse transcriptase p51 subunit



I375	T376	T377	E378	S379	I380	K388	F389	K390	I393	Q394	E399	T400	W401	W402	Y405	W406	Q407	W410	I411	E412	E413	V417	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	Q428	LEU	GLU	LYS	GLU	ILE	PRO	VAL	GLY	ALA	GLU	THR	PHE												
L303	A304	E305	N306	R307	E308	I309	L310	K311	E312	P313	V314	H315	G316	V317	Y318	Y319	D320	P321	S322	K323	D324	E328	K331	Q332	T338	Y339	Q340	Q343	E344	F345	F346	L349	K350	T351	R356	M357	R358	G359	A360	H361	T362	N363	D364	V365	K366	Q367	L368	T369	E370	A371	V372	Q373	K374				
T240	V241	Q242	P243	I244	V245	L246	P247	E248	K249	D250	S251	W252	T253	V254	I257	Q258	V261	G262	K263	W266	A267	S268	Q269	I270	Y271	P272	G273	I274	K275	V276	R277	Q278	L279	G280	K281	L282	L283	R284	G285	T286	K287	A288	L289	P290	E291	W292	I293	P294	L295	T296	E297	L298	E299	A299	E300	L301	K302
P170	K173	Q174	P175	N176	D177	Y183	M184	D185	D186	L187	Y188	S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	E204	L205	R206	L209	G213	L214	T215	T216	P217	D218	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PRO	PHE	LEU	TRP	MET	G231	Y232	E233	L234	H235	P236	D237	K238	W239				
I94	P95	H96	P97	A98	K101	K102	K103	K104	T107	V108	V111	G112	Y115	F116	S117	V118	D121	F124	R125	K126	Y127	T128	A129	F130	T131	I132	N136	N137	E138	T139	P140	G141	I142	R143	Y144	L149	P150	Q151	G152	W153	K154	G155	S156	F160	Q161	S162	I167	L168	E169								

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.91Å 69.04Å 104.33Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.80) 94.4 (30.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.312 0.256 , 0.304	Depositor DCC
R_{free} test set	1995 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CP9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/4483	1.08	35/6094 (0.6%)
2	B	0.62	0/3488	1.11	31/4740 (0.7%)
All	All	0.56	0/7971	1.09	66/10834 (0.6%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	LYS	N-CA-C	12.18	128.30	110.28
1	A	53	GLU	N-CA-C	9.70	124.16	110.68
1	A	227	PHE	N-CA-C	9.62	123.23	110.53
2	B	358	ARG	N-CA-C	7.92	127.68	110.80
1	A	13	LYS	CA-C-N	7.77	129.56	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4419	314	0
2	B	3392	0	3418	195	0
3	A	27	0	16	8	0
All	All	7786	0	7853	499	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

The worst 5 of 499 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:HG22	1:A:363:ASN:H	1.12	1.15
2:B:65:LYS:HE3	2:B:72:ARG:HD2	1.24	1.08
1:A:92:LEU:HD23	1:A:93:GLY:H	1.16	1.07
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.19	1.04
1:A:424:LYS:HD2	1:A:426:TRP:HE1	1.22	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/560 (95%)	442 (83%)	51 (10%)	38 (7%)	1	2
2	B	407/440 (92%)	334 (82%)	47 (12%)	26 (6%)	1	3
All	All	938/1000 (94%)	776 (83%)	98 (10%)	64 (7%)	1	2

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	137	ASN
1	A	141	GLY
1	A	225	PRO
1	A	230	MET

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/500 (96%)	455 (95%)	25 (5%)	21	53
2	B	373/400 (93%)	351 (94%)	22 (6%)	18	48
All	All	853/900 (95%)	806 (94%)	47 (6%)	19	51

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	68	SER
2	B	184	MET
2	B	95	PRO
2	B	151	GLN
2	B	216	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	GLN
2	B	147	ASN
2	B	136	ASN
2	B	151	GLN
1	A	334	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CP9	A	561	-	30,31,31	1.77	6 (20%)	41,45,45	1.49	6 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CP9	A	561	-	-	4/8/8/8	0/5/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	CP9	C14-N17	6.08	1.52	1.44
3	A	561	CP9	C2-N3	2.71	1.40	1.37
3	A	561	CP9	C22-C21	2.20	1.43	1.39
3	A	561	CP9	C13-C14	2.09	1.43	1.39
3	A	561	CP9	C9-C4	2.09	1.42	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	CP9	C21-N17-C18	-5.74	104.31	106.48
3	A	561	CP9	C11-C10-N3	3.12	118.54	113.46
3	A	561	CP9	C26-C18-N19	-2.94	121.07	124.80
3	A	561	CP9	C14-N17-C18	2.57	130.40	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	CP9	C22-C21-N17	2.26	134.65	130.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

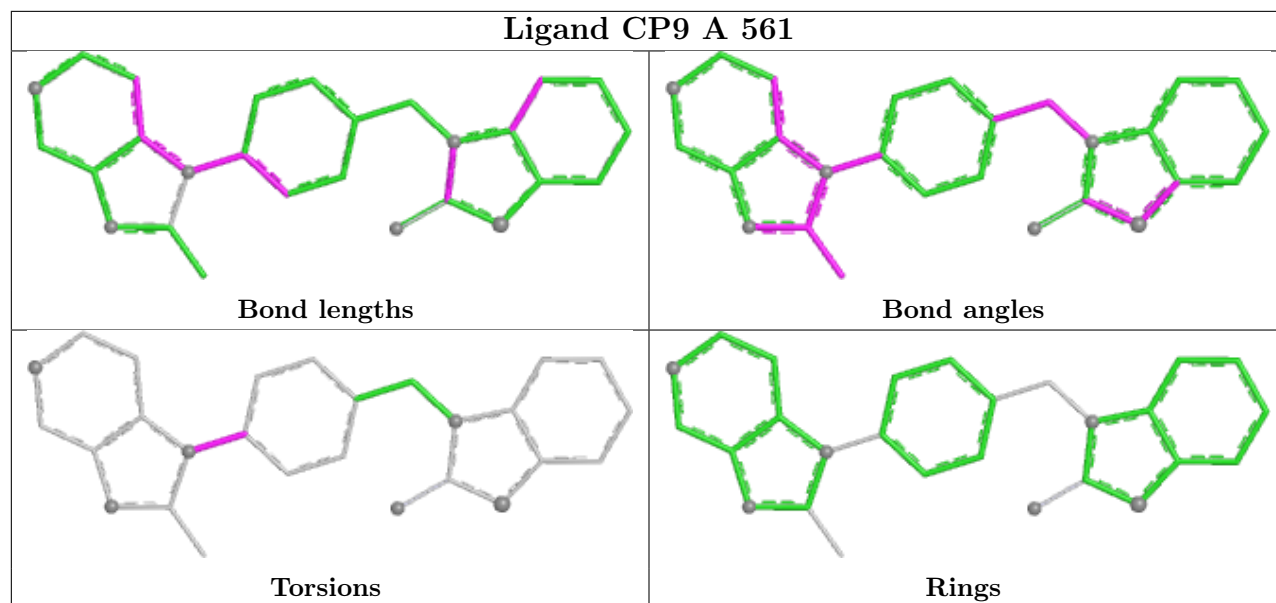
Mol	Chain	Res	Type	Atoms
3	A	561	CP9	C13-C14-N17-C18
3	A	561	CP9	C13-C14-N17-C21
3	A	561	CP9	C15-C14-N17-C18
3	A	561	CP9	C15-C14-N17-C21

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	CP9	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	535/560 (95%)	1.09	99 (18%) 3 2	12, 59, 95, 107	0
2	B	411/440 (93%)	0.65	71 (17%) 4 3	4, 38, 99, 105	0
All	All	946/1000 (94%)	0.90	170 (17%) 3 3	4, 53, 98, 107	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	LEU	6.1
1	A	140	PRO	5.9
2	B	423	VAL	5.4
2	B	421	PRO	5.2
1	A	290	THR	5.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

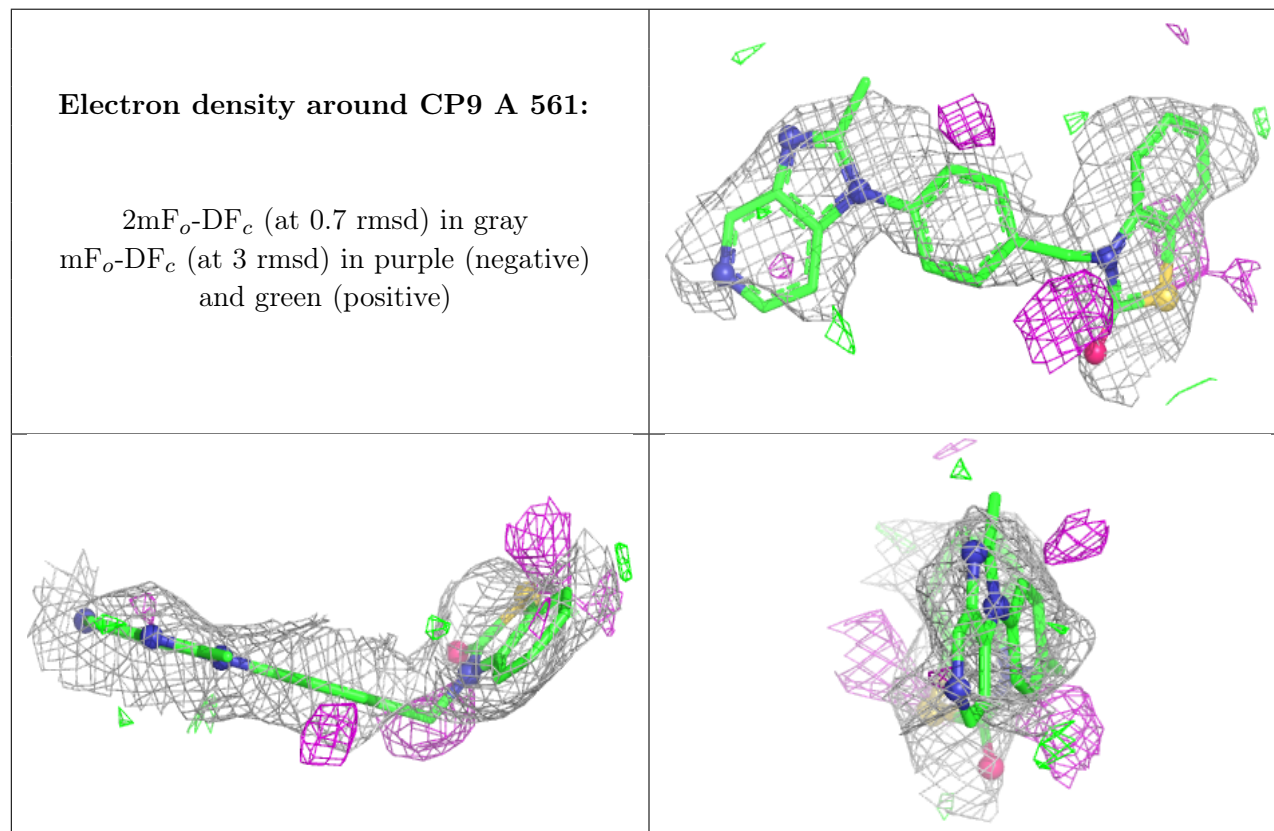
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CP9	A	561	27/27	0.73	0.20	62,68,73,74	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.